Tuning the electronic and magnetic properties of β_{12}-borophene

Adeleh Vatankhahan[1]
Tayebeh Movlarooy[1], Aran Garcia-Lekue[2,3]

[1] Shahrood University of Technology, Shahrood,Iran
[2] Donostia International Physics Center(DIPC), Donostia-San Sebastian, Spain
[3] IKERBASQUE, Basque Foundation for Science, Bilbao,Spain

a.vatankhahan@shahroodut.ac.ir

In last years, enormous research has been focused on two-dimensional (2D) nanomaterials due to their attractive physical properties and various technological applications. Recently, two-dimensional (2D) boron sheets named as borophene have been synthesized on silver surfaces [1-2]. Borophene exhibits various structural polymorphs, all of them metallic and highly anisotropic. However, pristine borophene is inherently non-magnetic, which limits its use for spintronic applications. Several approaches can be used to induce magnetic properties in borophene. For example, the adsorption of 3d transition metals (TM) or the patterning of borophene into 1D strips, named as borophene nanoribbons (BNRs) [3-4].

In this work, by using density functional theory (DFT), we investigate the changes in the electronic and magnetic properties of one of the polymorphs of borophene, called β_{12}, when TMs are adsorbed on it. Our calculations show that the electronic structure and the magnetic properties of borophene can be tuned by 3d TM atom adsorption, as shown in Figure 1. Based on the results for TM adsorption on extended β_{12}, the electronic transport properties of pristine and TM-doped β_{12}-BNRs will be explored. Our findings will be useful for the design of future borophene based spintronic devices.

References

[1] Mannix, A. J. *et al*. Science 350, 1513 (2015).
[2] Wang, H. F. *et al*. New J. Phys. 18, 073016 (2016).
[3] Sevinçli, H. *et al.* Phys. Rev. B 77 195434 (2008).
[4] Sahar Izadi .S. *et al.* Nanomicro Lett. 10 (2018).

Figures

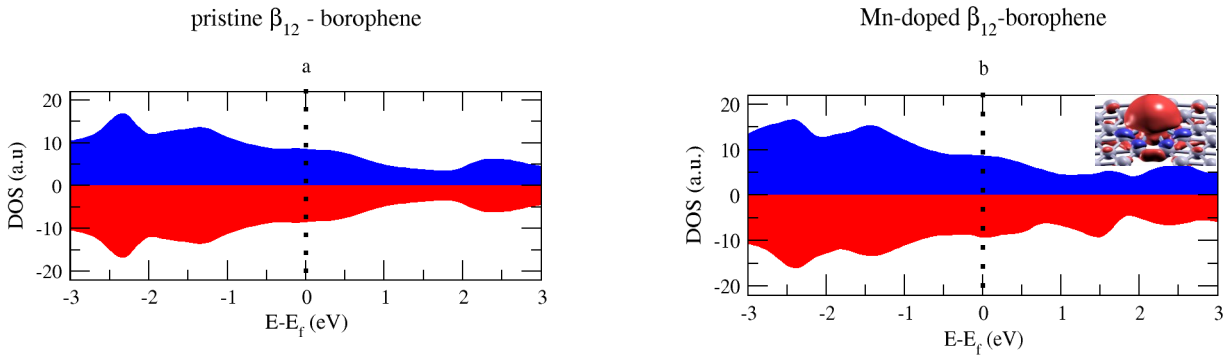

Figure 1. Density of states (DOS) of (a) pristine and (b) Mn doped borophene. The inset in (b) shows the spin density ($\rho\uparrow - \rho\downarrow$) isosurface distribution (0.0005eV/Å^3)